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Phase equilibria of multifunctional associating molecules: Measurements and modelling on hydroxybenzoic and phenilpropenoic acids

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Numerous molecules in the food, chemical and pharmaceutical industries present complex chemical structures with different functional group substitutions. Many of these groups such as hydroxyl, amine and carboxyl can form hydrogen bonds. To adequately describe the phase equilibria of these complex chemicals, models able to take into account association effects are required. Still, for model development and evaluation, experimental data on some representative systems are needed.

In this work, new experimental measurements and literature data were combined to develop a methodology to model the phase equilibria of phenolic acids using the Cubic-plus-Association (CPA) equation of state.

Solid-liquid equilibria of hydroxybenzoic acids such as gallic, salicylic, syringic and protocatechuic acids and phenilpropenoic acids such as trans-cinnamic, ferulic, coumaric and caffeic acids were measured from 288 K up to 323 K using the analytical shake-flask and a synthetic DSC method. Particular attention was given to aqueous solubilities. Besides solubility data, the melting properties (fusion enthalpies and temperatures) were also determined by DSC. The corresponding acid dissociation constants were determined by potentiometry.

A new methodology to obtain the associating energies and volumes of the different associating groups will be presented, and it will be demonstrated that the extent of hydrogen bonding is the dominant effect on the solubility of these compounds.

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